Hydrodynamic Modelling and Granular Dynamics

Peter Dybdahl Hede

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1st edition

ISBN 87-7681-172-7

Contents

Introduction to hydrodynamic modelling and granular dynamics

The present text introduces hydrodynamic modelling principles in the context of batch wet granulation and coating systems and it reviews the latest achievements and proposals in the scientific literature in this field. The text concerns primarily the Eulerian and the Lagrangian modelling technique. In accordance with some of the latest published Ph.d. thesis in the field of hydrodynamics modelling, the Lagrangian technique is divided into a soft-particle and a hard-sphere approach. The text further presents some of the latest trends and results from the growing field of applying Computational Fluid Dynamics and Discrete Element Modelling in the field of modelling fluid bed granulation processes. Further, a number of other granule dynamic modelling principles including the Finite Element and Monte Carlo techniques are introduced.

The text is aimed at undergraduate university or engineering-school students working in the field of mathematical or chemical and biochemical engineering. Newly graduated as well as experienced engineers may also find relevant new information as emphasis is put on the newest scientific discoveries and proposals presented in recent years of scientific publications. It is the hope that the present introductory text will be helpful to the reader – particularly in the early stages of the process of working with hydrodynamics in a granulation context. The comprehensive literature list may also hopefully be an inspiration for further reading.

I alone am responsible for any misprints or errors and I will be grateful to receive any critics and/or suggestions for further improvements.

Copenhagen, September 2006

Peter Dybdahl Hede

1 Hydrodynamic modelling and granular dynamics in respect to fluid bed processing

As it has been emphasised elsewhere (e.g. Hede, 2006b), a lot of research in fluid bed processing has focussed on modelling and understanding of the separate growth mechanisms associated with agglomeration. Much of this understanding of these separate mechanisms has been integrated into population balance models as it was presented in Hede (2006c). The available population balance models almost never take into account the hydrodynamic properties and influence on the fluid bed process, although the nature and detailed knowledge of fluidisation must be regarded as a prerequisite for precise modelling – especially when it comes to scaling of fluid bed processes. Hydrodynamic modelling of fluid bed systems seeks to include the effect of fluidisation although this approach is somewhat different from the population balance approach[1]. A hydrodynamic approach to fluid bed systems is a fairly new discipline that has developed in the last five to ten years due to the enormous increase in computer processing power and algorithm development. It is nevertheless a difficult but promising discipline being a prerequisite for discrete element modelling and computational fluid dynamic modelling which are both subjects to be presented in the present chapter.

Hydrodynamics is fluid dynamics applied to liquids, and as the bed load is fluidised in the fluid bed vessel during processing, *hydrodynamics* is often used as a term rather than the more general term *fluid dynamics*[2]. As with other typical fluid dynamic problems, a fluid bed hydrodynamic problem often involves the calculation of various properties for the fluidised particles such as velocity, pressure, density and temperature as function of space and time. The system consisting of the fluidised solid particles and the fluidising gas is often treated as a two-phase gas-solid flow system (Goldschmidt, 2001 and Goldschmidt et al., 2003). Modern approaches by Goldschmidt (2001) reduce this simplification by treating the fluid bed system as a multiphase system, which allows a detailed hydrodynamic modelling of the fluid phase of top-spray fluid beds. The description of such systems seeks in any case to account for the inherent complexity of dense gas-particle flows, which in its turn can be related to particle-particle and particle-wall interactions as well as gas-particle interactions (Goldschmidt, 2001). Hydrodynamic modelling is rarely combined with mass transfer or chemical/physical reactions and mechanisms as first attempts by Samuelsberg & Hjertager (1996) strongly indicate the prior need for valid and well-proven hydrodynamic models.

On an overall scale, there are basically two types of hydrodynamic models being the Eulerian models[3] and the Lagrangian models of which the first is commonly known as Computational Fluid Dynamic models (CFD) and the latter is commonly referred to as Discrete Element Models (DEM)[4]. Both types consider the gas phase as a continuum but there are quite a few differences in the modelling approaches and assumptions. The following sections will briefly introduce the basic principles and differences. An in-depth treatment of fluidised bed hydrodynamics and granular dynamics of two-phase flows should be found in Hoomans (1999) and Goldschmidt (2001).

1.1 Eulerian models

In Eulerian models the gas and the solid phases are treated as interpenetrating phases, and the theory behind such models is basically an extension of the classical kinetic theory that takes non-ideal particle-article collisions and gas-particle drag into account (Goldschmidt, 2001). In this scheme, collections of particles are modelled using continuous medium mechanics. The solid particles are generally considered to be identical having a representative diameter and density, meaning that the particle phase is volume averaged (Taghipour et al., 2005 and Depypere, 2005). The general idea in formulating such a multi-fluid model is to treat each phase as an interpenetrating continuum and therefore to construct integral balances of continuity, momentum and energy for both phases with appropriate boundary conditions and jump conditions for the phase interfaces. Since such a resulting continuum approximation for the solid phase has no equation of state and obviously lacks variables such as viscosity and normal stress, certain averaging techniques and assumptions are required to obtain a momentum balance for the solid phase (Pain et al., 2001).

Although constitutive relations according to the kinetic theory of particle flow have been incorporated into recent models (e.g. Gidaspow et al., 2004 and Chiesa et al., 2005), pure CFD models for fluid bed granulation still suffer from the fact that the contact between fluid, particles and boundary surfaces is not considered explicitly with respect to particle inertia and the mechanical properties of the particles. This limits the ability of CFD multiphase models to adequately represent particle-particle and fluid-particle interactions thereby reducing the accuracy of the prediction of both the fluid and the particle dynamics (Fan et al., 2003 and Sun, 2002). This inaccuracy can be overcome by explicit calculations of the particle contact mechanics in a particle-scale reference frame using a Lagrangian approach as it will be presented below. Considering the required computational power and complexity, gas-particle flow fields calculated with the multi-fluid interpenetrating approach of the Eulerian granular multi-phase model is still a fast method to calculate flow fields, as it is well known from simple particle systems as spray-drying and conveying systems etc. Due to the obvious need for accounting precise particle level properties into fluid bed hydrodynamic models, pure Eulerian CFD models[5] must be regarded as inappropriate even in an industrial context. Hydrodynamic fluid bed scaling attempts on empty vessel basis are often based on Eulerian models (e.g. Krishna & van Baten, 2001 and Cooper & Coronella, 2005) but the models often turn out to be inaccurate when particles are being processes. Recent attempts by e.g. Depypere (2005) and Lettieri et al. (2003) quite clearly illustrates that future development in the field of hydrodynamic fluid bed modelling should be concerned with Lagrangian principles rather than Eulerian.

1.2 Lagrangian models – Discrete Element Methods

The Lagrangian approach may be seen as an extension of the Eulerian, in that Lagrangian model describes the solids phase at particle level and the gas phase as a continuum. In the two-phase flow situation the Newtonian equations of motion for each individual particle are solved with inclusion of the effects of particle collisions and forces acting on the particles by the gas (Goldschmidt, 2001). That is, Newton's law of motion is simultaneously solved for a large number of particles either in a computational unit cell with periodic boundaries or on a computational domain representing the entire fluid bed vessel or its subset. In general the following equations are solved (Cameron et al., 2005):

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i \tag{1.1}$$

and

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \mathbf{M}_i \tag{1.2}$$

in which m_i is the particle mass, $\mathbf{v}_i$ is the velocity vector, t is time, I_i is the moment of inertia, $\boldsymbol{\omega}_i$ is the angular velocity vector, $\mathbf{M}_i$ is the net torque vector and $\mathbf{F}_i$ is the net force vector acting on particle i. The net force vector $\mathbf{F}_i$ is often written as the sum of three contributions (Cameron et al., 2005):

$$\mathbf{F}_i = \mathbf{F}_i^{H} + \mathbf{F}_i^{P} + \mathbf{F}_i^{E} \tag{1.3}$$

where $\mathbf{F}^H$ is the force due to fluid-particle interactions also known as the *drag force*, $\mathbf{F}^P$ is the force due to particle-particle interactions during collisions and $\mathbf{F}^E$ is a force acting on the particle due to an external field being e.g. the gravitational field. $\mathbf{F}^E$ is sometimes completely ignored and $\mathbf{F}^H$ is often estimated from empirical equations, and many discrete element approaches involves different assumptions and expressions for the net force vector in equation 1.3 (Goldschmidt et al., 2004).

Besides obviously being far more precise than the Eulerian models, such discrete particle models do not require additional closure equations for the suspended particulate phase since they compute the motion of every individual particle, taking collisions and external forces acting on the particles directly into account (Goldschmidt, 2001). The Lagrangian approach may roughly be divided into two groups being the soft particle and the hard-sphere approach, both of which will be briefly introduced below.

1.2.1 Hard-particle models

In hard-sphere models the particles are assumed to interact through instantaneous, binary collisions. A sequence of collisions is processed one collision at the time in order of occurrence (Hoomans, 1999, Hoomans et al., 2000 and Tsjui et al., 1993). Hard-sphere models are also referred to as event driven models since a sequence of collisions is processes in which all particles are moved until the next collision occurs. Particle collision dynamics are described by collision lays, which account for energy dissipation due to non-ideal particle interaction by means of the empirical coefficients of normal and tangential restitution and coefficient of friction (Goldschmidt, 2001). The dissipative particle interaction in particle media makes these systems significantly different from molecular systems where energy associated with collision always is conserved. This means that energy has to be continuously supplied to the particle system in order to keep the particles in motion. This can for instance be achieved by applying a shear rate through proper choice of boundary conditions as suggested by Campbell & Brennen (1985). It has become common to choose the collision particle partners and sequences based on the relative approach velocity (Hoomans et al., 1996 & 2000).

Based on work by Hoomans (1999), Goldschmidt (2001) and Goldschmidt et al. (2003) developed a hard-sphere discrete particle model for gas-fluidised beds which captures the principles of basic two dimensional hard-sphere modelling well. This model computes the motion of every individual particle as well as droplet in the system considering the gas phase as a continuum. Micro-scale processes such as particle-particle collisions, droplet-particle coalescence and agglomeration are taken into account by simple closure models. Distinction is made between three types of entities being dry particles, wetted particles and droplets. All three types are assumed to be spherical, and encounters are detected as soon as contact occurs at a point on the line joining the centres of the two entities. In addition, six types of encounters are distinguished: encounters among dry particles described by hard-sphere collision laws from mechanics; Droplet-droplet encounters described by hard-sphere collisions laws as well, as they are assumed to be repulsive for atomised liquid droplets with a typical radius of 50 μm, colliding with small mutual differences; Encounters between droplets and dry or wetted particles, described as coalescence; Encounters between dry or wetted particles and a wall, described by hard-sphere collision laws; Encounters between droplet and walls, resulting in removal of the droplet from the simulation and last; Encounters between a wetted particle and another particle, leading to either rebound described by hard-sphere collision laws or agglomeration. Which of the two situations that occurs depends on the odds of the particles hitting each other on a wet spot (Goldschmidt et al., 2003). It is further assumed that a new particle entity is formed at the position of the centre of mass of the original entities upon coalescence as it is sketched in figure 1.

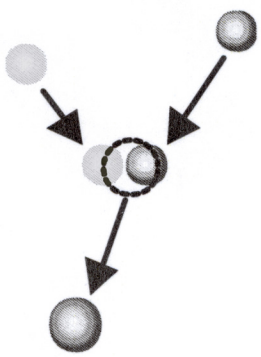

Figure 1: Repositioning and merging of particles upon coalescence or agglomeration (Goldschmidt et al., 2003).

Mass, momentum and volume of the new entities are conserved and transferred to the newly formed particle, where after the original entities are excluded from the simulation. In case of coalescence, the area on the newly formed particle covered by liquid depends on the original particle size, the size of the droplet and a defined minimum liquid layer thickness as sketched in figure 2.

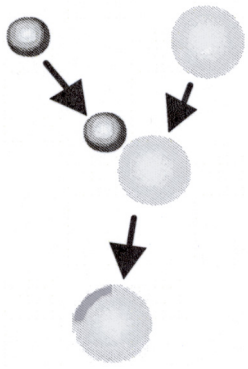

Figure 2: Liquid layer formation upon coalescence (Goldschmidt et al., 2003).

In case of agglomeration, the wetted area available for subsequent agglomeration is reduced by the projected area of the smallest particle, to account for liquid bridge formation and the masking of the wetted surface, which cannot be reached anymore because the newly agglomerated particle is in the way. This is sketched in figure 3.

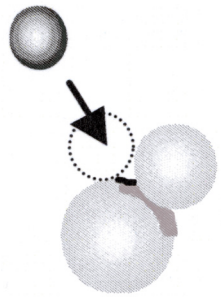

Figure 3: Masking of wetted surface for subsequent agglomeration (Goldschmidt et al., 2003).

Although inclusion of liquid and gas inside the pores is taken into account for agglomerates containing more than three primary particles in the model by Goldschmidt et al. (2003), the model does however not account for particle deformation, liquid spreading, breakage of droplets and agglomerates, and is further limited by the two-dimensional geometry. Even so, the simulation using the simple two-dimensional Goldschmidt model is only possible for 50,000 granules at the time thereby being only comparable to experimental data from laboratory-scale fluid beds. This clearly illustrates the need for increased computational power if the hard-sphere principles should be used for any industrial purposes, and also indicates why the hard-sphere approach has first been used within the last ten to fifteen years although the principles were introduced originally in the late fifties. In recent modelling attempts, hard-sphere models are mainly concerned with rapid particle flow[6] (Lian et al., 1998) and the majority of the latest discrete element attempts concerns the soft-particle approach.

1.2.2 Soft-particle models

The soft-particle approach differs from the hard-particle approach in that it treats interparticle collisions as a continuous process that takes place over a finite time. In such models the particles are assumed to undergo deformation during their contact, where the contact forces are calculated from a simple mechanical analogy involving a spring, a dashpot and a friction slider as the normal and tangential component of forces are expressed as the sum of forces due to the springs and dashpots, and the normal and tangential velocities are expressed in terms of the relative velocity prior to collision (Gera et al., 1998). Such inter-particle bond models are particular suitable for the modelling of impact breakage of pre-existing agglomerates which undergo some sort of brittle fracture (Thornton & Cismocos, 1999). This is why the majority of discrete element simulations of agglomerate strength use the soft-particle approach as mentioned in the previous section. The principle of the linear spring-dashpot model is sketched in figure 4.

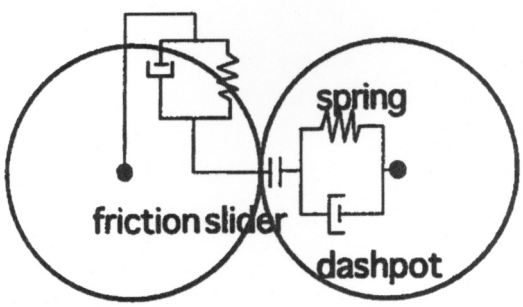

Figure 4: Contact force model for soft particle modelling (Gera et al., 1998).

With soft-particle simulations, the interactive forces exerted on each particle are computed as continuous functions of the distance between contiguous particles and are based on physically realistic interaction laws. Soft-particle models are also referred to as time driven models as all particles are moved over a certain period of time where after the collision dynamics are computed from the particle overlaps. In case a particle is in contact with several other particles, the resulting contact force follows from the addition of binary contributions (Goldschmidt, 2001). Compared to the hard-sphere principle this approach is computationally intensive and requires even higher computational demands than the hard-sphere simulations, but does as a clear advantage provides information on the structure and dynamics of particular materials including details of positions, velocities, forces and energy partitions (Lian et al., 1998). This makes soft-particle modelling useful in the simulation of the deformation and breakage of agglomerates. In soft-particle simulations of coalescence, agglomerates are modelled as assemblies of primary particles, which often are assumed to be spherical and elastic.

In a representative example of a soft-particle coalescence model, Lian et al. (1998) developed a model in which each agglomerate comprised 1000 randomly packed primary particles with the interparticle interactions modelled as the combination of the solid-solid contact forces and the principles for the pendular liquid bridges presented in Hede (2006a). It is assumed that the binding liquid present at particle junctions completely wets the particles. With this set-up, the coalescence of two randomly packed agglomerates each consisting of 1000 primary particles was studied at different impact velocities. Initially 1000 primary particles were randomly generated in each of two specified spherical regions that were not able to touch. Centripetal gravity fields were then applied to the two spherical regions in order to bring the particles together and, depending on the size of this field, the regions would impact each other at different velocities. When two primary particles collided, a pendular liquid bridge was assigned to that contact. The kinematic energy was eventually dissipated due to the retarding effect of the viscous liquid bridges. When equilibrium was achieved, the centripetal gravity was removed. Pendular liquid bridges then held the particles together. The impact simulation was implemented for a range of initial relative velocities between the two agglomerates and for different interstitial binder fluid viscosities, and for each collision, the simulation was continued until a major proportion of the initial kinetic energy was essentially dissipated. Examples of computer simulated wet agglomerates after impact at a velocity of 2.0 m/s with different interstitial viscosities ranging from 1 mPa s to 100 mPa s can be seen in figure 5.

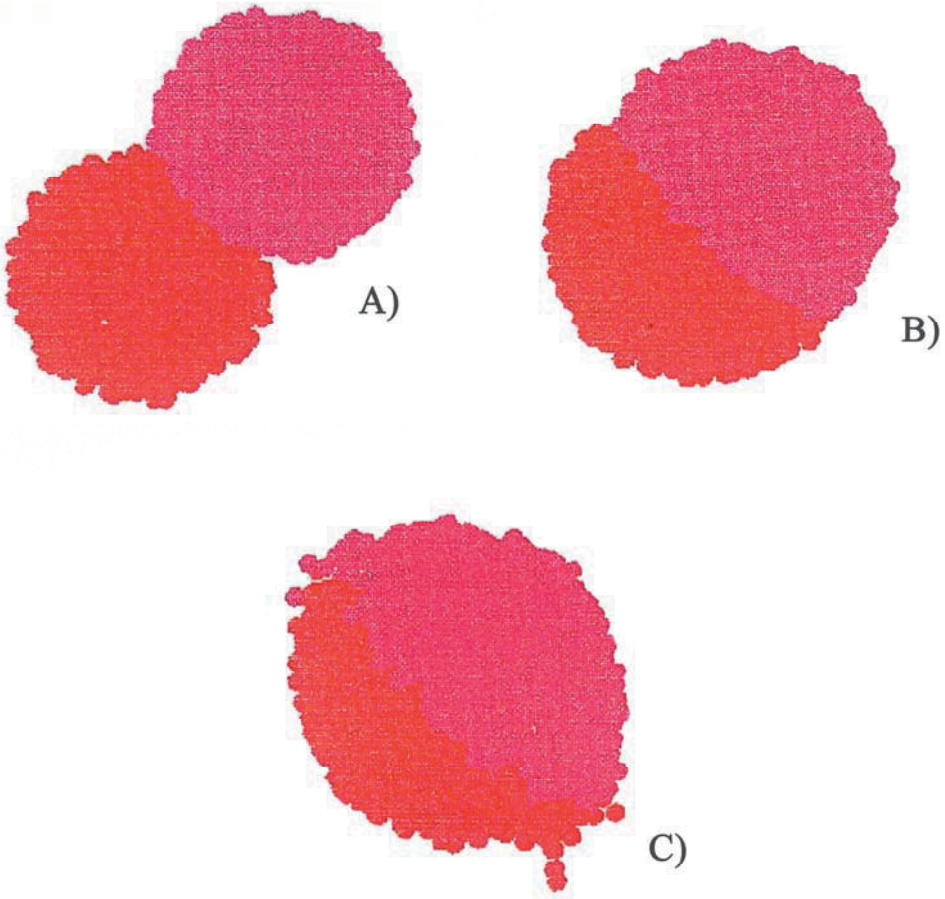

Figure 5: Computer simulations of agglomeration.

Visualisations of computer simulated pendular state wet agglomerates after impact at a velocity of 2.0 m/s for interstitial viscosities of: (a) 100 mPa s, (b) 10 mPa s, (c) 1 mPa s (Lian et al., 1998).

The results by Lian et al. (1998) illustrate the possibilities regarding the simulation of the coalescence situation at particle level, but with the large computer processing time even for the binary collision situation it is obvious that such an approach cannot easily be extended to model the high number of particles inside a commercial fluid bed. Even if it at some point will be possible due to the development in computational processing power, agglomeration in fluid beds cannot be fully understood or modelled just by treating the binary coalescence situation, as it has been emphasised in Hede (2005 & 2006b). More advanced algorithms must be developed and implemented into soft-particle programs in order to account for the random nature of particle collisions in real fluid bed. Soft-particle simulation is nevertheless a promising tool for studying the effect at particle level of changing some of the physical parameters. Once the program is set up, changes can be made infinitely as only the processing time sets the limit with the present available computers. E.g. have the previously mentioned simulations by Lian et al. (1998) indicated that during binary collision the dominant energy dissipation is the viscous dissipation, except when the fluid viscosity is relatively small. These tendencies would have been extremely time consuming to extract from experimental data.

1.2.3 Summing up on Lagrangian modelling

Since Lagrangian models describe particle motions in detail, it is expected that these models show closer resemblance with experimental results than with the Eulerian models. However, a direct comparison between hard- or soft-sphere models and experiments has not been made so far mainly because of the large number of particles that is required to justify the application of the continuum approach on one hand, and the limited number of particles that can be handled by the discrete element models on the other hand. Further complications arise from the fact that a rigorous comparison can only be made if the discrete element models account for the full three-dimensional motion of the particles as a two-dimensional modelling of the particle collision dynamics has proven to be too restrictive (Hoomans, 1999). This further strongly increases the required number of particles and consequently the computational demands. The number of particles that can be accounted for in such models is a generic but serious limiting factor in any of the present Lagrangian models. Even with modern computers, present models cannot account for more than 10^6 particles, which is several orders of magnitudes lower than that encountered in industrial fluid beds. Rough estimations based on Moores law for computer processing development estimate that models accounting for all three dimensional particles in industrial scale fluid beds will not be within reach in the coming ten to fifteen years (Webopedia, 2005 and Michales, 2003).

1.3 Other granular dynamic modelling principles

Besides the Eulerian and Lagrangian approaches, other principles have been applied for particle systems similar to fluid beds. These principles will only be briefly introduced, as the reported simulations of fluid bed systems using these techniques are extremely limited in number.

1.3.1 Monte Carlo techniques

Another method to study many particle systems is the Monte Carlo[7] technique. A Monte Carlo simulation is a mathematical experiment in which the behaviour of a system is simulated incorporating stochastic behaviour modelled using a randomness generator to vary the behaviour of the system (Kaye, 1997). This principle has been applied to several particle technology disciplines as reviewed by Wauters (2001). Regarding fluid bed granulation, Rosato et al. (1996) have applied Monte Carlo techniques. In their simulations a new overlap-free particle configuration was generated in each processing step. The change in the system energy was then calculated and if the change was negative, the new configuration was accepted. If the system energy on the other hand increased, the new configuration was accepted with a probability obtained from a statistical distribution based on the change in energy. With this method it was possible to simulate segregation and collision phenomena in agitated systems as fluid beds.

The Monte Carlo technique is capable of predicting steady state conditions being e.g. equilibrium conditions and for this purpose it has certain advantages over other hydrodynamic simulations techniques. As time is not a variable in Monte Carlo simulations, a Monte Carlo step can only be linked to an actual time step by means of calibration, which is a difficult task. In practice this means that Monte Carlo simulations of particle dynamics is not possible without input of a-priory knowledge. This is an obvious disadvantage when simulating agglomerating systems as the likelihood of permanent coalescence is closely related to time (Hoomans, 1999). Recent fluid bed hydrodynamic simulations seldom use the Monte Carlo principles although the technique has been applied elsewhere in fluid bed modelling. E.g. have Hapgood et al. (2004) used Monte Carlo techniques for the simulation of atomised droplets impacting the fluidised particle bed.

1.3.2 Finite Element scheme

The finite element method is well known from simple transport problems but has recently been applied to fluid bed systems. The principle involves discretising a large domain into a large number of small elements (which is often chosen to be triangles), developing element equations, assembling the element equations for the whole domain and then solve the assembled equations. The finite element discretisation of the governing differential equations is based on the use of interpolating polynomials to describe the variation of a field variable within an element. This makes finite element method well suited for irregular geometries and heterogeneous materials. Recent advances in finite element programs makes it possible to perform simulations that account for dynamic transport, heat and mass transfer, axial and radial dispersion, temperature and pressure variations and different hydrodynamic flow regimes, which is a prerequisite for fluid bed simulations (Wang & Sun, 2003). Results from catalytic fluid bed systems by Mahecha-Botero et al. (2005) seems promising as the models requires fewer assumptions than any of the principles presented earlier in this chapter. Modern finite element models can be reasonable accurate predictors of particle stresses if the bulk properties used as constitutive parameters are measured, but the finite element method struggles in general with boundary conditions when the bed particle material is fluidised at high fluidisation velocities (Bell, 2005). As it is the case with other simulation techniques, finite element model requires large processing times.

Summary

The hydrodynamic approach on fluid bed granulation is a rapid growing field and a number of the most used available techniques for modelling the fluid bed particle-gas flow system have been presented in the previous sections. As in other parts of the chemical engineering science, there is a tendency to try to simulate and to model the hydrodynamics rather than to build uniform test equipment or try to conduct detailed experiments. With the complex behaviour of fluidisation and the chaotic phenomena of particles trajectories, the reasons for this are obvious. As the computational processing capacity is roughly doubled each 18 month, the boundaries for what is possible and what is not, are in continuous motion.

Effective modelling of solid-fluid flow requires methods for adequately characterising the discrete nature of the solid phase and representing the interaction between solids and fluids. CFD multiphase models such as the Euler method address the problem within a continuum framework. In continuum models, contact between gas, particles and boundary surfaces is not considered explicitly with respect to particle inertia and mechanical properties. This limits the ability of CFD multiphase models to adequately represent particle-particle and fluid-particle interactions, and may therefore reduce the accuracy of the prediction of both the fluid and the particle dynamics. Despite the modelling challenges, applications of CFD to model hydrodynamics continues to develop as it has many advantages including design optimisation and scale-up of systems. Some of the correlations used in the present models however remain to be empirical or semi-empirical. As a result, the model and its parameters must be validated against experimental data obtained at similar scale and process configurations. The limitation of CFD models to represent particle-level interactions can be overcome by explicit calculation of the particle contact mechanics in a particle-scale reference frame using a Discrete Element (Lagrangian) approach such as the hard-sphere or soft-sphere principle.

As it was presented earlier, a discrete element algorithm is basically a numerical technique, which solves engineering problems that are modelled as a large system of distinct interacting general shaped (deformable or rigid) bodies or particles that are subject to gross motion. Engineering problems that exhibit such large scale discontinuous behaviour as a particle fluid bed cannot be solved with a conventional continuum based procedure such as the Finite Element Method, although new expansions of the Finite Element technique in fact seems to have somewhat solved these issues. The discrete element procedure is used to determine the dynamic contact topology of the bodies. It accounts for complex non-linear interaction phenomena between bodies and numerically solves the equations of motion. Since the DEM is a very computationally intensive procedure, many existing computer codes are limited to model either two-dimensional or small three-dimensional problems that employ simple particle geometries. A general problem with Discrete Element modelling is that the simulation either concerns mechanical properties such as breakage and attrition or concerns agglomeration, but never accounts for all phenomena in the same model.

Despite the different theories and techniques associated with the presented hydrodynamics modelling principles, validation is a general problem with any of the simulation techniques. There are only few research groups around the world that work specifically in the field of fluid bed hydrodynamic modelling and most of the equipment, that is used to validate the simulation results, have been built by the research group itself. This means that published results are difficult to reproduce and further exploit and expand. As hydrodynamic modelling generally is very time-consuming and further requires advanced equipment such as high-speed cameras and specially designed fluid beds allowing the fluidisation behaviour to be recorded, hydrodynamic modelling will probably for some time on continue to be a part of fluid bed modelling only for an exclusive number of research groups around the world. As a sum-up, table 1 presents some of the most important advantages and disadvantages associated with the different hydrodynamic modelling techniques presented in the present chapter.

	CFD	DEM		Other granular modelling techniques	
	Eulerian	Hard-sphere	Soft-sphere	Monte Carlo	FE
Advantages	CFD is a fast method to calculate flow fields at any fluid bed scale, and is far from being as processing time demanding as the other techniques. CFD provides a detailed understanding of flow velocity distribution, weight loss, mass and heat transfer. CFD makes it possible to fast evaluate geometric equipment changes with much less time and cost than would be involved in laboratory or pilot plant testing. A whole range of CFD commercial programs are available making the simulation coding part fairly straightforward. CFD can be applied in the process of scaling equipment as the CFD models are based on fundamental physics and are thereby scale independent.	High precision of the particle dynamics as the Newtonian equations of motion for each individual particle are solved with inclusion of the effects of particle collisions and forces acting on the particles by the gas. A larger number of particles can be included into the hard sphere models than is possible in soft-sphere models.	High precision of the particle dynamics as the Newtonian equations of motion for each individual particle are solved with inclusion of the effects of particle collisions and forces acting on the particles by the gas. Soft-particle simulation is a promising tool for studying the effect at particle level of changing some of the physical parameters involved in the granulation process. Theoretical particle level models may be validated using the soft-particle approach as numerous variations in the physical/ chemical parameters may be simulated relatively fast once the simulation program is set up. Soft-sphere models are well suited for studying the modelling of impact breakage of pre-existing agglomerates.	The Monte Carlo algorithm is incorporated into many program languages thereby making the coding part of the simulation fast and reliable. The principles behind the Monte Carlo techniques are easy to follow, and the principles may be used elsewhere in the granulation process – e.g. in the prediction of the wetting behaviour of the atomised droplets on the fluidised particle bed. Monte Carlo models are capable of predicting steady state conditions.	The Finite Element method is well suited for irregular geometries and heterogeneous materials. FE models require fewer assumptions than any of the other principles. A range of commercial FE programmes is available, making the coding part of the simulation fast and reliable.

Disadvantages	Knowledge of the equation of state for the particles is needed a-priori. Results from empty vessel CFD simulations may not readily be used when particles are being processed. In CFD models for fluid bed granulation, contacts between fluid, particles and boundary surfaces are not considered explicitly with respect to particle inertia and the mechanical properties of the particles. Due to the obvious need for accounting precise particle level properties into fluid bed hydrodynamic models, CFD models must be regarded as inappropriate for simulating particle systems.	Hard-sphere models lack precision in fluid bed processes without rapid particle flow. Although hard-sphere simulations can yield both size and composition distribution of granules, it is generally not suitable for realistic representation of the granule microstructure (i.e. the internal distribution of primary solids, binder and porosity of the granule). Microstructure is an important property especially in the case with enzyme granules as it determines the release rate of the enzyme ingredient from the granule. Present models are only capable of accounting for 50,000 granules at the time, thereby making simulations comparable only to experimental data from laboratory scale fluid beds.	Soft-particle simulations struggle with high computational processing demands. Detailed information of binary collisions is far from being representative of the situation inside a fluid bed. Although soft-sphere simulations can yield both size and composition distribution of granules, it is generally not suitable for realistic representation of the granule microstructure (i.e. the internal distribution of primary solids, binder and porosity of the granule). Microstructure is an important property especially in the case with enzyme granules as it determines the release rate of the enzyme ingredient from the granule.	Limited available literature makes Monte Carlo simulations yet an unproven technique. A-priori knowledge from experiments is needed as input in the models. As time is an important parameter in the granulation process, time scale statements should be incorporated into Monte Carlo models before any advanced simulation of the fluid bed granulation process should be reliable.	Limited available literature makes Finite Element simulations yet an unproven technique. Problems with boundary conditions means that FE until recently has been unsuited for simulations of systems in random motion. Large processing time even with modern computers.

Table 1: Advantages and disadvantages associated with the hydrodynamic modelling techniques presented in the text.

Table of symbols

Nomenclature		Unit (SI-system)
a	Internal coordinate	-
a'	Material constant	Dimensionless
a_d	Projected area of liquid binder droplets	m^2
a_{AE}	Fitting parameter	Dimensionless
a_n	Projected area of a nucleus granule	m^2
$\dot{A}$	Powder flux	m^2/s
A^*	Contact area between colliding granules	m^2
b	Internal coordinate	-
b_{AE}	Fitting parameter	Dimensionless
c	Cohesivity of dry particle mass	N/m^2
$d_{air\ distrib\ pl.}$	Air distribution plate diameter	m
d_b	Gas bubble diameter	m
d_{bed}	Fluidised bed diameter	m
d_d	Liquid droplet diameter	m
$d_{d,rel}$	Relative liquid droplet diameter	m
d_p	Particle diameter	m
$d_{orifices}$	Pitch orifice diameter	m
$d_{sp/sp}$	Interaction parameter of two spheres	m
d_v	Equivalent diameter of particles	m
d_{vessel}	Fluid bed vessel diameter	m
e	Particle coefficient of restitution	Dimensionless
E	Young modulus	N/m^2
E^*	Granule Young modulus	N/m^2
E_{elu}	Elutriation rate	-
$f_1(\mathbf{x}, \mathbf{r}, t)$	Average number density function	-
f_{bi}	Bi-variant average number density function	-
$f_{initial}$	Initial average number density function	-
f_{tetra}	Tetra-variant average number density function	-
$F_{pend.,bound.}$	Pendular force in the “boundary” method	N
$F_{pend.,eq\ sph.}$	Pendular force between two equally sized spheres	N
$F_{pend.,gorge.}$	Pendular force in the “gorge” method	N
F_{vis}	Viscous force	N
$\mathbf{F}_i$	Net force vector acting on particle i	-
$\mathbf{F}_i^{\mathbf{H}}$	Drag force vector	-
$\mathbf{F}_i^{\mathbf{E}}$	Force vector accounting for external fields	-
$\mathbf{F}_i^{\mathbf{P}}$	Force vector accounting for particle-particle interactions	-
g	Gravity	m/s^2

$G(\mathbf{x}, \mathbf{r}, t)$	Rate of growth by layering	-
G_s	Mass flux of particles	m^2/s
$h(\mathbf{x}, \mathbf{r}, t)$	Net generation rate of particles	-
h_0	Binder layer thickness covering colliding granules	m
h_a^+	Birth of particles due to aggregation	-
h_a^-	Death of particles due to aggregation	-
h_{asp}	Characteristic length scales of surface asperities	m
h_b^+	Birth of particles due to breakage	-
h_b^-	Death of particles due to breakage	-
h_{bed}	Bed height	m
H	Separation distance between two spheres	m
i	Summation parameter	-
I_i	Moment of inertia	-
J	Nucleation ratio	Dimensionless
k	Proportionality constant	-
k´	Proportionality constant	-
k_{cn}	Coordination number	Dimensionless
K_a	Nucleation area ratio	Dimensionless
L	Characteristic length of particles	m
L_{bed}	Fluid bed length from distributor plate to exhaust exit	m
L_{slr}	Length scale ratio	Dimensionless
m	Mass	kg
$m(\mathbf{x})$	Mass of a particle of internal state **x**	
m_{aggl}	Agglomerate mass	kg
m_{bed}	Bed load	kg
m_{harm}	Harmonic mean granule mass	kg
$\dot{m}_{nozzle\ air}$	Spray rate from the nozzle	kg/s
$\dot{m}_{spray}$	Air flow rate through the nozzle	kg/s
$\mathbf{M}_i$	Net torque vector	-
n_{fi}	Flow index	Dimensionless
$n(\mathbf{x}, \mathbf{r}, t)$	Actual number density	-
$\dot{n}_0$	Nucleation rate	No. of particles/s
$N(\mathbf{r}, t)$	Average total number of particles	-
N_T	Total number of particles	-
N_{T0}	Initial total number of particles	-
p	Summation number	Dimensionless
P	Pressure	Pa
$P(\mathbf{x},\mathbf{r}\|\mathbf{x}',\mathbf{r}')$	Probability density function	-
q	Discretisation number	Dimensionless
r	Radius	m
r_{aggl}	Radius of an agglomerate	m

r_{def}^{*}	Critical radius of an agglomerate after which def. occurs	m
r_{harm}	Harmonic mean granule radius	m
r_{neck}	Pendular bridge neck radius	m
$\bar{r}_g$	Mean granule size	m
$\bar{r}_{g_0}$	Initial mean granule size	m
r_{neck}	Pendular bridge neck radius	m
$\mathbf{r}$	External coordinate vector	-
$\mathbf{r}'$	External coordinate vector	-
R	Radius	m
R_p	Particle radius	m
s_{max}	Maximum pore liquid saturation	Dimensionless
S	Distance	m
S_c	Saturation at transition funicular/capillary state	Dimensionless
S_d	Dry coating material feed rate	-
S_f	Saturation at transition pendular/funicular state	Dimensionless
S_{sat}	Amount of saturation	Dimensionless
St_{def}	Stokes deformation number	Dimensionless
St_{def}^{*}	Critical Stokes deformation number	Dimensionless
St_v	Viscous Stokes number	Dimensionless
St_v^{*}	Critical viscous Stokes number	Dimensionless
S_w	Wetting saturation	Dimensionless
S(q)	Summation function	-
$S_{Kolmogorov}$	Kolmogorov entropy	bits/s
t	Time	s
t_{coat}	Coating time	s
u	Granule velocity	m/s
u_0	Initial granule collision velocity	m/s
U	Fluidisation velocity	m/s
U_{br}	Bubble rise velocity for a fluid bed	m/s
U_{mf}	Minimum fluidisation velocity	m/s
U_s	Superficial gas velocity	m/s
$\mathbf{v}_i$	Velocity vector	-
v	Particle volume internal coordinate	-
$\bar{v}$	Average particle volume	m^3
v_L	Liquid binder volume internal coordinate	-
$\dot{V}$	Volumetric spray rate	m^3/s
V_{aggl}	Agglomerate volume	m^3
V_{bridge}	Liquid bridge volume	m^3
$V_{\mathbf{r}}$	Volume of external coordinates	-
$V_{\mathbf{x}}$	Volume of internal coordinates	-
w	Granule volume parameter in coal. kernel expression	-

w^*	Critical average granule volume	-
w_{mr}	Mass ratio of liquid to solid	Dimensionless
W	Spray zone width	m
x	Internal coordinate vector	-
x´	Internal coordinate vector	-
x	Coordinate	m
y	Coordinate along the width of the spray zone	m
Y(**r**,t)	Continuous phase vector	-
Y_d	Plastic yield stress	N/m^2
z	Counting number	Dimensionless

Greek

β	Coalescence kernel	-
β_0	Rate constant	-
β_{dt}	Aggregation probability in time interval dt	-
β_{id}	Coefficient of interphase drag	Dimensionless
β^*	Coalescence kernel expression	-
δ	Dimensionless bubble spacing	Dimensionless
δ_{pdef}	Extent of permanent plastic deformation	Dimensionless
μ_f	Coefficient of internal friction	Dimensionless
μ_{mean}	Mean in the Gaussian distribution	m
σ_f	Macroscopic shear stress at failure	Pa
σ_n	Macroscopic normal stress	Pa
σ_{width}	Standard deviation	m
$\sigma_{t,f}$	Funicular bridge static tensile strength	N/m^2
$\sigma_{t,p}$	Pendular bridge static tensile strength	N/m^2
$\sigma_{t,c}$	Capillary bridge static tensile strength	N/m^2
$\sigma(\dot{\gamma})$	Characteristic stress in an agglomerate	N/m^2
σ_y	Yield stress/strength	N/m^2
τ_c	Average particle circulation time	s
τ_d	Droplet penetration time	s
ψ_a	Dimensionless spray flux	Dimensionless
$\psi_n(y)$	Dimensionless nuclei distribution function	Dimensionless
ψ_n	Dimensionless spray number	Dimensionless
ζ	Particle shape factor (sphericity)	Dimensionless
λ	Dimensionless parameter in the dynamic strength eq.	Dimensionless
φ	Half filling radius	°
Θ	Contact angle	°
ν	Poisson ratio	Dimensionless
$\nu(\mathbf{x}',\mathbf{r}',\mathbf{Y},t)$	Average number of particles formed from break up	-
ε	Particle voidage (void fraction)	%
$\varepsilon_{longitudinal}$	Longitudinal extension strain	Dimensionless
ε_{min}	Minimum porosity	%
ε_{trans}	Transverse contraction strain	Dimensionless
$\bar{\varepsilon}_g$	Mean granule porosity (void fraction)	%
γ_{lv}	Interfacial surface tension between liquid and vapour	N/m
$\dot{\gamma}$	Shear rate	s^{-1}
ρ	Density	kg/m^3
ρ_b	Binder liquid density	kg/m^3

ρ_g	Granule density	kg/m^3
ρ_p	Particle density	kg/m^3
η_{app}	Apparent viscosity	kg s /m
η_{liq}	Liquid (binder/coating) viscosity	kg s /m
$\boldsymbol{\omega}_i$	Angular velocity vector	-
Ω_H	Hounslow discretisation parameter	-
Ω_r	Domain of external coordinates	Dimensionless
Ω_x	Domain of internal coordinates	Dimensionless

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Endnotes

1. Some of the newest studies in granulation modelling do however indirectly include population balance equations as well as discrete element simulation techniques (e.g. Gantt & Gatzke, 2005).
2. Fluid dynamics is the sub discipline of fluid mechanics that studies fluids in motion. Fluids are specifically gases and liquids. Commonly, fluid dynamics is divided into sub disciplines being aerosol dynamics (the study of gases) and hydrodynamics (the study of fluids and thereby fluid like systems) (Wikipedia, 2005).
3. Also known as "Continuum models" or "Eulerian-Eulerian models" (Goldschmidt, 2001 and Taghipour et al., 2005).
4. Actually Computational Fluid Dynamics is formally the overall term for all hydrodynamic modelling (and thereby also for DEM), but it has become common to refer to other terms when granular dynamics is involved (Hoomans, 1999).
5. An excellent review of available commercial CFD programmes can be found in Xia & Sun (2002).
6. Hoomans (1999) has compared the results of a soft-sphere model to those of a hard-sphere model and found that, provided that the spring stiffness was high enough, the difference in bed hydrodynamics between the two types of models were very small. This further supports the soft-particle approach for fluid bed modelling.
7. The term "Monte Carlo" refers in general to any technique of statistical sampling employed to approximate solutions to quantitative problems such as dice tosses or the chance that two particles in a bulk sample will collide (Webopedia, 2005).